Effect of pressure on distillation

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Fenske equation

For a simple situation, the Fenske equation gives the minimum number of trays (even Wikipedia has this...) as a function of the relative volatility. The distillate mole fraction is xd and the bottoms mole fraction is xb.

In[49]:= `fenske = Log[ ( xd / (1 - xd) (1 - xb) / xb)] / Log[α]`

Out[49]= $$\frac{Log\left[\frac{(1-xb)\ xd}{xb\ (1-xd)}\right]}{Log[\alpha]}$$

In[51]:= `Plot[fenske /. {xd → .99, xb → .01}, {α, 1.1, 4},`
  `  AxesLabel → {" α -- relative volatility", "minimum trays"}]`

Out[51]=
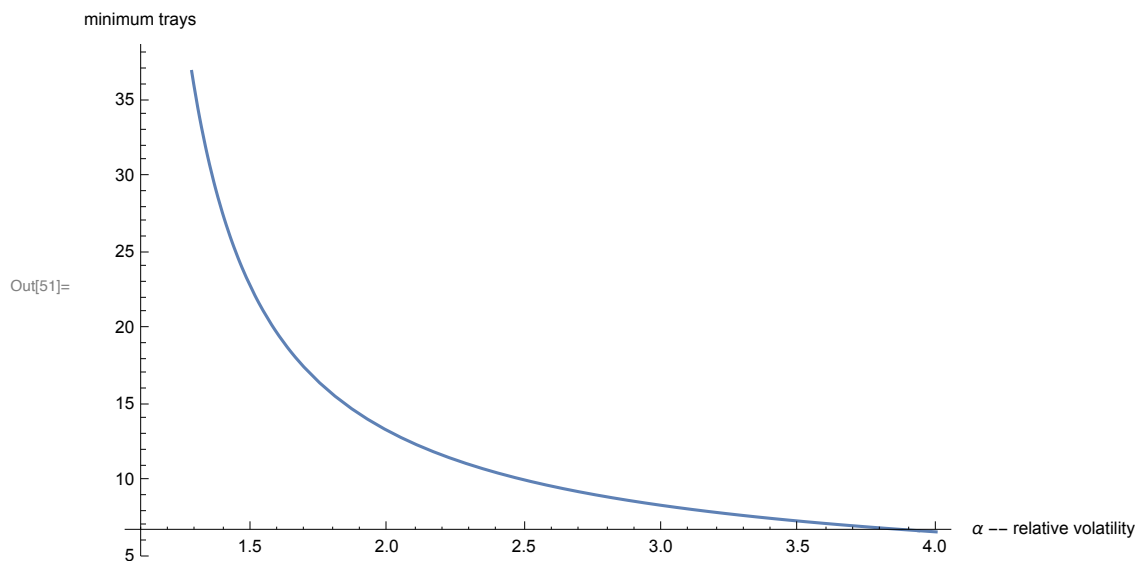
An example of α, toluene, hexane

T is in C.

In[8]:= `Psat1[T_] := (1 / 760) * 10 ^` $\left(6.95087 - \frac{1342.31}{T + 219.187}\right)$`; (*toluene*)`

`Psat2[T_] := (1 / 760) * 10 ^` $\left(6.91058 - \frac{1189.64}{T + 226.28}\right)$`; (*n hexane*)`

Raoult's law

For Raoult's law, the relative volatility is just the ratio of vapor pressures. Note that the total pressure divides out, but as P increases, T must increase and stay above the bubble point.

In[52]:= `Plot[Psat2[T] / Psat1[T], {T, 25, 250}, AxesLabel → {"T - Celsius", "α"}]`

Out[52]=
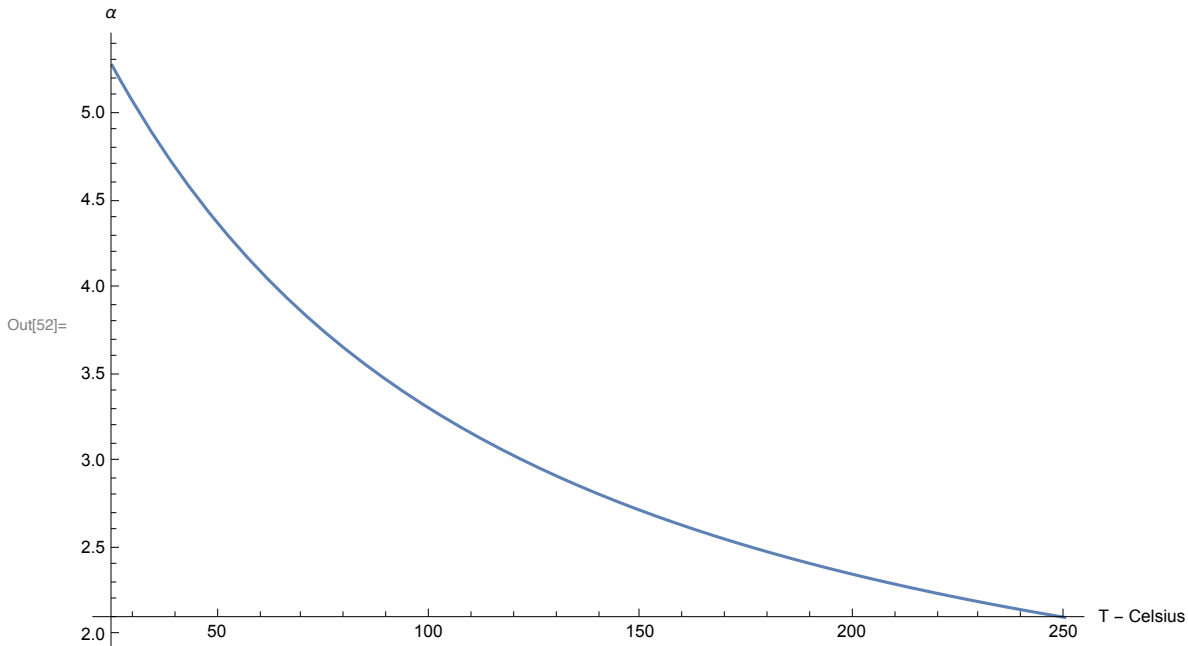
We see that as T increases, the relative volatility decreases significantly. Does this occur all of the time... some other day.

We will do a bubble point calculation below, but the Fenske equation tells us that the minimum number of trays will vary as

In[55]:= `Plot[fenske /. {α → Psat2[T] / Psat1[T], xd → .99, xb → .01},`
`  {T, 25, 250}, AxesLabel → {"T-- Celsius", "minimum trays"}]`

Out[55]=
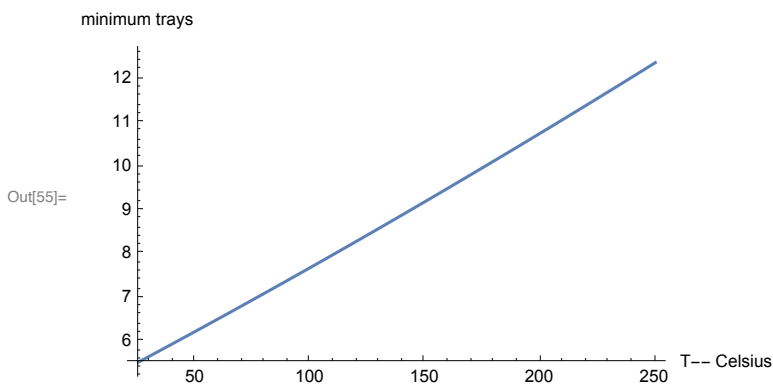
Since the actual trays will be some factor, we see that the number of trays would be expected to double over this temperature range.
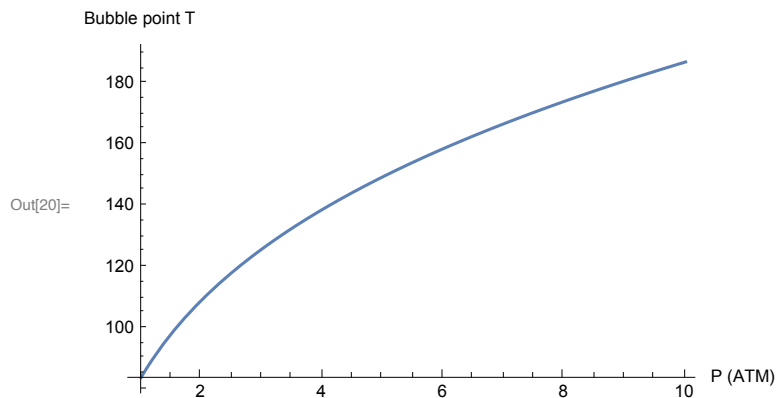
Bubble point, Raoult's Law

We will pick a total pressure and find the bubble point T. Use a x=.5 feed.

In[16]:= **eq1 = ptotal == .5 Psat1[T] + .5 Psat2[T]**

Out[16]= $\text{ptotal} == 0.0263158 \times 2^{3.95087 - \frac{1342.31}{219.187 + T}} \times 5^{5.95087 - \frac{1342.31}{219.187 + T}} + 0.0263158 \times 2^{3.91058 - \frac{1189.64}{226.28 + T}} \times 5^{5.91058 - \frac{1189.64}{226.28 + T}}$

In[20]:= **Plot[T /. FindRoot[eq1, {T, 25}], {ptotal, 1, 10},**
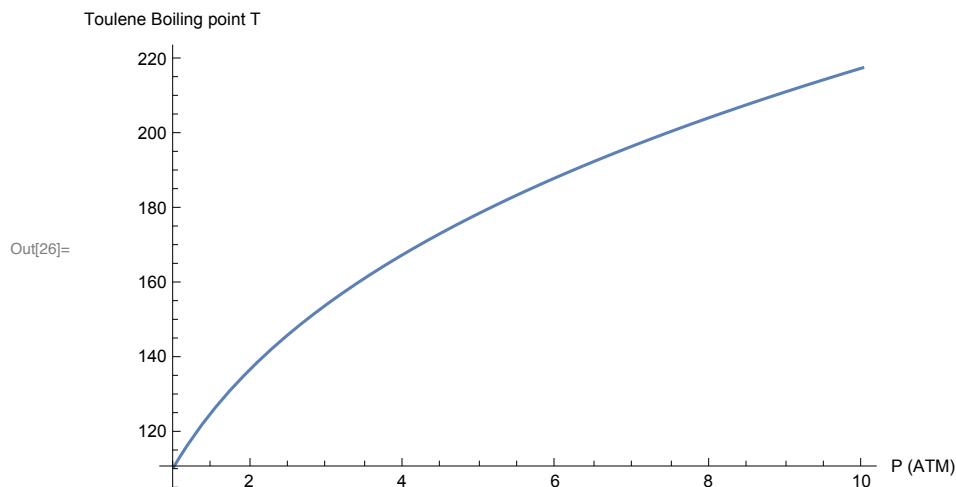   **AxesLabel → {"P (ATM)", "Bubble point T"}]**

Out[20]=

Or check the boiling point of toluene

In[25]:= **bp1 = ptotal == Psat1[T]**

Out[25]= $\text{ptotal} == \frac{1}{19} \times 2^{3.95087 - \frac{1342.31}{219.187 + T}} \times 5^{5.95087 - \frac{1342.31}{219.187 + T}}$

In[26]:= **Plot[T /. FindRoot[bp1, {T, 25}], {ptotal, 1, 10},**
   AxesLabel → {"P (ATM)", "Toulene Boiling point T"}]
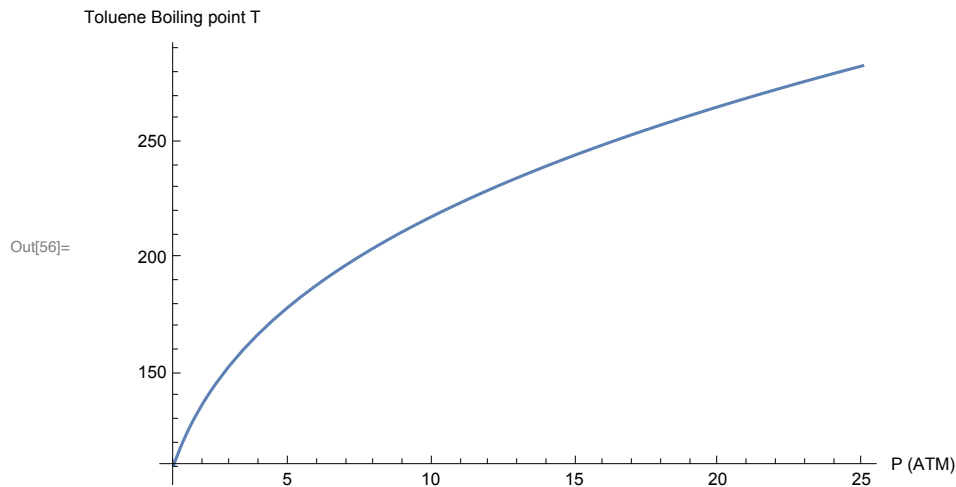
Out[26]=

Now back to distillation scaling

We know Raoult's law is a poor approximations as P increases past a couple of ATM. However, save fixing it for another day...
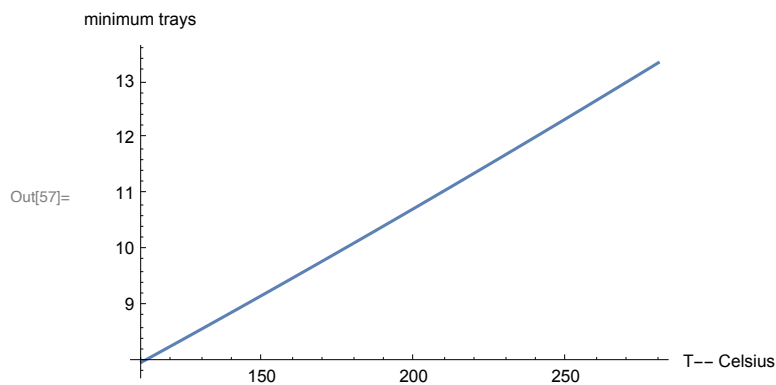
Temperature range to check...

In[56]:= `Plot[T /. FindRoot[bp1, {T, 25}], {ptotal, 1, 25},`
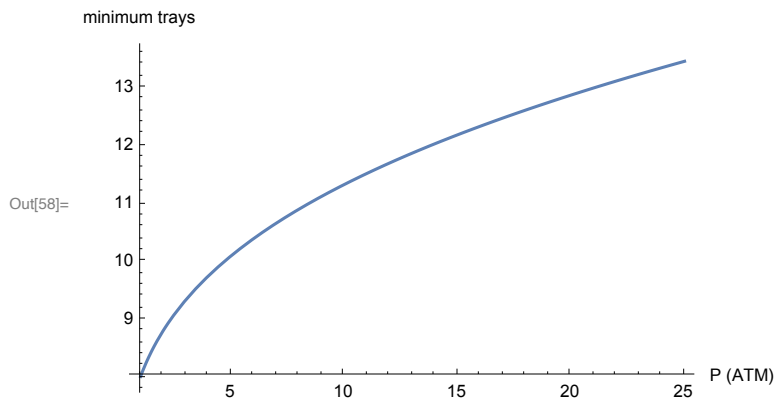   `AxesLabel → {"P (ATM)", "Toluene Boiling point T"}]`

Out[56]=

Minimum Trays... (Fenske eq.)

In[57]:= `Plot[fenske /. {α → Psat2[T] / Psat1[T], xd → .99, xb → .01},`
    `{T, 110, 280}, AxesLabel → {"T-- Celsius", "minimum trays"}]`

Out[57]=

So the minimum trays would vary from ~8 to ~13 at the highest pressure.

In[58]:= `Plot[(fenske /. {α → Psat2[T] / Psat1[T], xd → .99, xb → .01}) /.`
`    FindRoot[bp1, {T, 25}][[1]], {ptotal, 1, 25},`
`  AxesLabel → {"P (ATM)", "minimum trays"}]`

Out[58]=

minimum trays

[Plot showing a curve rising from around 8 at P=1 to about 13.5 at P=25, with y-axis values 9, 10, 11, 12, 13 and x-axis values 5, 10, 15, 20, 25 labeled P (ATM)]

Minimum reflux...

The minimum reflux directly reflects energy costs. How does this change?

The simplest relation for minimum reflux is the "Underwood Equation". A reference for this is King's book: "Separation Processes", McGraw Hill, 1971, but there is probably a 2nd edition and the Under-wood equation is probably in many texts...

$$\frac{(x_D\ D\ /\ (x_F\ F)\ -\ \alpha\ (1-x_D)\ D\ /\ ((1-x_F)\ F))}{\alpha - 1}$$

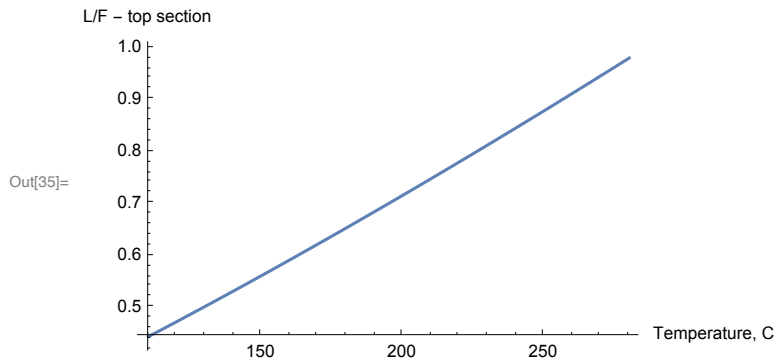We pick a saturated liquid feed for simplicity, a 50 - 50 initial mixture and .99 xd and xb

In[29]:= `LminslashF = (.99 - α .01) / (α - 1)`

Out[29]= $\dfrac{0.99 - 0.01\,\alpha}{-1 + \alpha}$

L is the liquid flow in the upper part of the column, LminslashF is L/F, where F is the (liquid) Feed.

In[35]:= `Plot[LminslashF /. α → Psat2[T] / Psat1[T], {T, 110, 280},`
`  AxesLabel → {"Temperature, C", "L/F - top section"}]`

Out[35]=

L/F – top section

In[31]:= `minRflux = (.99 - α .01) / (α - 1) 2`

Out[31]= $\dfrac{2\,(0.99 - 0.01\,\alpha)}{-1 + \alpha}$

In[36]:= `Plot[minRflux /. α → Psat2[T] / Psat1[T], {T, 110, 280},`
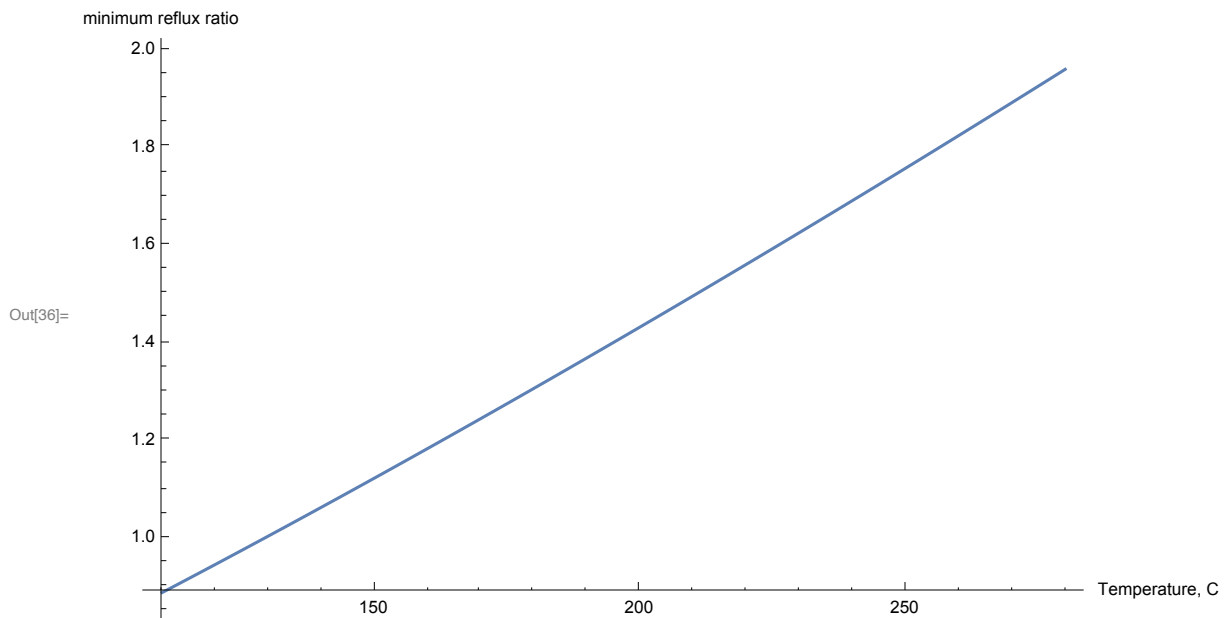`  AxesLabel → {"Temperature, C", "minimum reflux ratio"}]`

Perhaps the standard "R" reflux ratio, which is "L" from here divided by D, which is the distillate product flow rate would be easier. F = 2 D for this idealized case...
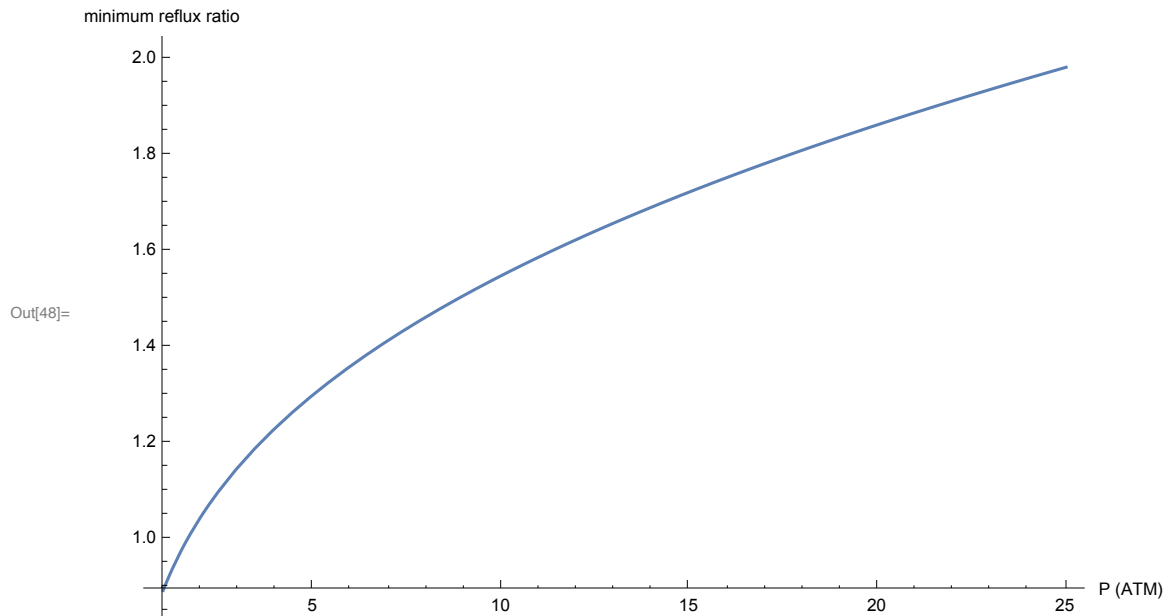
Out[36]=

minimum reflux ratio

In[48]:= `Plot[(minRflux /. α → Psat2[T] / Psat1[T]) /. FindRoot[bp1, {T, 25}][[1]],`
`{ptotal, 1, 25}, AxesLabel → {"P (ATM)", "minimum reflux ratio"}]`

Out[48]=

So the reflux ratio and hence the energy requirements will vary by about a factor of 2. For commodity chemical processing, even a few % of energy savings is important!